

THE DIFFUSION OF RADON SHAPE*

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Abstract

Almost thirty years ago, D.G. Kendall [8] considered diffusions of shape induced by independent Brownian motions in Euclidean space. In this paper, we consider a different class of diffusions of shape, induced by the projections of a randomly rotating labelled ensemble. In particular, we study diffusions of shapes induced by projections of planar triangular configurations of labelled points onto a fixed straight line. That is, we consider the process in Σ_1^3 (the shape space of labelled triads in \mathbb{R}^1) that results from extracting the “shape information” from the projection of a given labelled planar triangle, as this evolves under the action of a Brownian motion in $\text{SO}(2)$. We term the thus defined diffusions Radon diffusions and derive explicit stochastic differential equations and stationary distributions. The latter belong to the family of angular central Gaussian distributions. In addition, we discuss how these Radon diffusions and their limiting distributions are related to the shape of the initial triangle, and explore whether the relationship is bijective. The triangular case is then used as a pivot for the study of processes in Σ_1^k arising from projections of an arbitrary number k of labelled points on the plane. Finally, we discuss the problem of Radon diffusions in general shape-space Σ_n^k .

Keywords: Single particle Biophysics; circular Brownian motion; D.G. Kendall’s shape theory; angular central Gaussian distribution; integral geometry; stochastic geometry; random processes of geometrical objects; Radon diffusion; Radon transform; singular value decomposition.

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1 Introduction

The study of the diffusion of the *shape* of a number of labelled points randomly moving in Euclidean space has been connected to the general theory of shape right from its outset. D.G. Kendall [8] introduced this area in studying the evolution of the shape of a given number of labelled points, as these independently perform Brownian motion in Euclidean space. He concluded that the shape performed itself a Brownian motion (after an appropriate time change). W.S. Kendall [10, 11] demonstrated that it is possible to employ computer algebra techniques to disentangle the study of such problems, and also proposed a diffusion model that relates to the *Bookstein theory of shape* [1] in the case of planar triangles. A dual problem was considered by Le [13], namely that of determining the characteristics of diffusions in pre-shape and pre-shape-and-size spaces that will induce Brownian motions on the resulting shape and shape-and-size spaces.

In this paper, we introduce a diffusion of shape induced by the projections of shape preserving diffusions of labelled points. What do we mean by this? The initial diffusion is the result of the action of a Brownian motion in $\text{SO}(2)$ on the vertices of a planar configuration of labelled points. Naturally, this sort of process leaves the shape of the configurations invariant. However, what we wish to consider is the shape of its projections on a line, which is constantly changing as $\text{BM}(\text{SO}(2))$ acts on the initial triangle. We call the

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resulting shape diffusions *Radon shape diffusions* as they are the shape-theoretic analogue of a random Radon transform (see section 3). Interestingly, in the case of Radon shape diffusions of labelled planar triangles, the stationary distributions are simple and of a known family, the central angular Gaussian family (section 4). The results from the triangular case set the scene for the study of the case of shape diffusions arising from projections of k labelled planar points.

A motivation for such an investigation comes from the field of biophysics, and in particular that of single particle electron microscopy (e.g. Glaeser [3], Glaeser et al. [4]). Biophysicists wish to learn about the structure of biological macromolecules, since this is intimately connected with their functional purpose. To this aim they use the electron microscope to image single particles (as opposed to crystalline structures) in aqueous environment. This method yields information on the projected structure of the particles. Since these particles are extremely small (in the realm of a few angstroms, $1 \text{ \AA} = 10^{-10}$ meters) it is impossible to rotate them at will so as to have a proper Radon transform (see section 3.1.). Instead, the projections obtained are at random angles, as these particles move around in their aqueous environment.

The paper is organized as follows. In section 2 we introduce some basic concepts along with notation, pertaining to the investigation of the shape of projections of planar triangles. In section 3.1. we recall the definition of the Radon transform and introduce the concept of a Radon process. We then proceed to study the shape of Radon diffusions arising from planar triangles in section 3.2., and obtain their stationary distributions in section 4. Section 5 considers a singular case (when all vertices of the “triangle” are collinear). The results on Radon diffusions for planar triangles are then “extended” to the case of general planar configurations in section 6. Finally, the paper closes with a discussion of the general setup (projections of \mathbb{R}^n -ensembles) and some concluding remarks, in section 7.

2 The Shape of a Projected Planar Triangle

In this section, we introduce the basic setup for our investigation along with the pertinent notation. Consider a labelled triangle on the plane, \mathbb{R}^2 , with vertices $\mathbf{a} = (x_a, y_a)^\top$, $\mathbf{b} = (x_b, y_b)^\top$ and $\mathbf{c} = (x_c, y_c)^\top$. We assume that there is no straight line that contains all three vertex vectors, so that we have a proper triangle. We represent this triangle by a matrix V , whose columns are the vertex vectors, so that using block notation,

$$V = \begin{pmatrix} \mathbf{a} & \mathbf{b} & \mathbf{c} \end{pmatrix},$$

with V a 2×3 matrix. As is implicit from our notation, the labels for the triangle vertices are $\{a, b, c\}$. Thus, order of the columns of V is important, as this “encodes” the label information (a permutation of the columns will analogously permute the labels). We will not be interested in any of the characteristics of V that have to do with location, scale or orientation. Thus, we may assume without loss of generality that the centroid of the triangle is 0 (the centre of gravity is at zero) and hence, the row sums of V are zero.

Suppose that we rotate the triangle V clockwise by an angle ϕ and then project it onto a straight line. Without loss of generality, we may assume the latter to be the x -axis. The projection $p(V, \phi)$ of the rotated triangle is essentially the 3-vector of x -coordinates of the ϕ -rotated vertex vectors

$$p(V, \phi) = \begin{pmatrix} u(\phi) \cdot \mathbf{a} \\ u(\phi) \cdot \mathbf{b} \\ u(\phi) \cdot \mathbf{c} \end{pmatrix} = \begin{pmatrix} x_a \cos \phi + y_a \sin \phi \\ x_b \cos \phi + y_b \sin \phi \\ x_c \cos \phi + y_c \sin \phi \end{pmatrix} = V^\top u(\phi),$$

where $u(\phi) := (\cos \phi, \sin \phi)^\top$ and “ \cdot ” denotes inner product. In the sequel, the notation $p(V, u(\phi))$ will be equivalent to $p(V, \phi)$. Although $p(V, \phi)$ is an element of \mathbb{R}^3 , we prefer to think of it as an arrangement of three points on the real line as we will be interested in the shape of such projections. However, it is useful to treat the ensemble as an ordered triplet, since it is this very order that implicitly provides the labels for the points.

We may notice that in order to describe the arrangement of the triplet, two points and knowledge of the centroid will suffice. Consequently, we may orthogonally transform the configuration so as to use only two points to parameterize it, since, by assumption, the centroid of the triplet $p(V, \phi)$ will be zero, regardless of

the angle ϕ . Such a transformation may be carried through by multiplying $p(V, \phi)^\top$ from the right with the matrix

$$Q = \begin{pmatrix} \frac{1}{\sqrt{3}} & -\frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{6}} \\ \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{6}} \\ \frac{1}{\sqrt{3}} & 0 & \frac{2}{\sqrt{6}} \end{pmatrix}. \quad (1)$$

In order to obtain the *shape* of the projected triple we must quotient out the group generated by translations, rotations and dilatations (quotienting out by the group generated only by translations and rotations provides the *shape-and-size* of the ensemble).

The effects of location are a priori removed by the assumption on the centroid of the triangle V . Furthermore, we recall that the rotation group on \mathbb{R} , $\text{SO}(1)$, is trivial, hence rotations have been quotiented out by degeneracy. Thus, only multiplying by Q^\top from the left yields the *shape-and-size*, S , of the projected triangle at angle ϕ :

$$S = Q^\top V^\top u(\phi).$$

Notice that since matrix multiplication is associative, it makes no difference whether we first orthogonally transform the triangle and then rotate and project it, or we first rotate and project it, and then orthogonally transform its projection. Although S is a 3-vector, it is essentially a two-dimensional object, since we may ignore the element of the triple that is identified with zero, so that $S = (S_1, S_2)^\top \in \mathbb{R}^2$. Hence, we will formally equate the 2×3 matrix $Q^\top V^\top$ with the 2×2 matrix Γ of its non-zero elements,

$$VQ = [\mathbf{0} \quad \Gamma^\top], \quad (2)$$

so that

$$S \equiv \Gamma u(\phi).$$

Finally, we obtain the shape σ of the projected triangle $p(V, \phi)$ upon scaling by the *size* $\|p(V, \phi)\| = \|S\| = (S_1^2 + S_2^2)^{\frac{1}{2}}$ of $p(V, \phi)$,

$$\sigma = \frac{Q^\top V^\top u(\phi)}{\|Q^\top V^\top u(\phi)\|} = \frac{\Gamma u(\phi)}{\|\Gamma u(\phi)\|} \in \mathbb{S}^1, \quad (3)$$

with \mathbb{S}^1 denoting the unit circle (we use the topology rather than the geometry notation). Notice that since $\sigma \in \mathbb{S}^1$ we may formally identify σ with $\arg(S_1 + iS_2) \in [0, 2\pi)$.

3 Radon Diffusions from Planar Triangles

We now entertain the situation in which the original triangle is randomly rotated as a result of certain “random shocks” and study the behaviour of the resulting projected size-and-shape process and the projected shape process. First, though, we make a short excursion to discuss the Radon transform and a stochastic extension.

3.1 The Radon Transform and Stochastic Analogues

The Radon transform was first introduced in 1917 by J. Radon [21] in terms of a purely mathematical question: do the integrals of a function over all possible manifolds of its domain completely determine this function?

Interestingly, Radon’s results remained unnoticed until the 1960’s, when their enormous practical significance started to emerge through the realisation of their central role in imaging problems. One may treat the Radon transform at different levels of abstraction (Helgason [6], Deans [2]). In the context of the present paper, the following definition is most appropriate:

Definition 1 (The Radon transform). Let $g : \mathbb{R}^{n+1} \rightarrow \mathbb{R}$ be a function of compact support. The Radon transform of g is a linear operator $\mathcal{R} : C_0(\mathbb{R}^{n+1}) \rightarrow C_0(SO(n+1) \times \mathbb{R}^n)$ defined by

$$(\mathcal{R}g)(A, x_1, \dots, x_n) := \int_{-\infty}^{\infty} g(A^\top \mathbf{x}) dx_{n+1},$$

for all $\mathbf{x} = (x_1, \dots, x_{n+1}) \in \mathbb{R}^{n+1}$ and $A \in SO(n+1)$, provided the integral exists.

The inversion of this transform is typically carried out through the use of Fourier transforms. Intuitively, the Radon transform maps the contours of a function in \mathbb{R}^{n+1} to the set of their projections (in terms of line integrals) onto every possible n -dimensional hyperplane. For example, the Radon transform of the density of a bivariate Gaussian distribution with diagonal covariance matrix $c\mathbf{I}$ is a fixed univariate Gaussian density, regardless of the straight line upon which we project it (by invariance under orthogonal transformations).

The relevance of the Radon transform to imaging problems is as follows. Suppose that instead of observing a three-dimensional object, we are able to observe its two-dimensional projections in a range of angles, and wish to reconstruct the former from the latter information. Then we may restate this problem as one of inverting a Radon transform. Problems of this nature can arise in such diverse fields as microscopy, astrophysics, geology and medical imaging (see Deans [2]). It is possible to envisage practical situations when the rotational aspect of the transform is both uncontrollable and stochastic (as in the single particle structural biology setup). In fact, one may consider scenarios where the rotations evolve in time as a stochastic process. With such possibilities in mind, one is motivated to define a random process analogue to the Radon transform. In the next paragraph we introduce such a setup within the context of D.G. Kendall's shape theory.

3.2 Shape-Theoretic Radon Diffusions

In the scenario we wish to consider, we want the rotation angles to vary continuously, so that a mathematically natural choice is to make them vary according to a Brownian motion modulo 2π . Let $\{\beta_t\}_{t \geq 0}$ be circular Brownian motion,

$$\beta_t = e^{iB_t} \quad \forall t \geq 0,$$

where $\{B_t\}_{t \geq 0}$ is standard Brownian motion in \mathbb{R} (we shall interchange $x + iy$ and $(x, y)^\top$ without special mention, when there is no danger of confusion). At each point in time, we rotate V according to β_t and obtain the shape-and-size and the shape of the projection $p(V, \beta_t)$,

$$S(p(V, \beta_t)) = QV^\top \beta_t \equiv \Gamma \beta_t \quad \text{and} \quad \sigma(p(V, \beta_t)) = \arg(S_1(t) + iS_2(t)),$$

where Γ is as in (2). Then, we show that

Theorem 1. Let V be a proper planar triangle and $\beta_t = e^{iB_t}$ be circular Brownian motion, where B_t is standard Brownian motion in \mathbb{R} . Then, the shape-and-size $S_t \equiv S(p(V, \beta_t))$ of the Radon process $\{p(V, \beta_t)\}$ evolves as Brownian motion on the ellipse $\mathcal{E}(\Gamma) = \{\mathbf{x} \in \mathbb{R}^2 : \mathbf{x}^\top (\Gamma \Gamma^\top)^{-1} \mathbf{x} = 1\}$, solving the Itô stochastic differential equation

$$dS_t = -\frac{1}{2} S_t dt + \Gamma A \Gamma^{-1} S_t dB_t,$$

where A is counterclockwise rotation by $\pi/2$.

We call the diffusion $\{S_t\}_{t \geq 0}$ a *Radon diffusion of shape and size*.

Proof. Since the triangle corresponding to V is proper, it must be that the matrix V has rank 2. This implies that Γ is of full rank. Hence, Γ transforms the unit circle to the ellipse $\mathcal{E}(\Gamma)$. Now, $S_t = \Gamma \beta_t$, so that the range of $\{S_t\}$ must be $\mathcal{E}(\Gamma)$, since the range of $\{\beta_t\}$ is the unit circle.

To see that $\{S_t\}$ performs Brownian motion on $\mathcal{E}(\Gamma)$, we consider the singular value decomposition of Γ ,

$$\Gamma = U \Lambda W^\top, \tag{4}$$

where U and W are 2×2 orthogonal matrices and $\Lambda = \text{diag}\{\lambda_1, \lambda_2\}$. Consider the action of $\Gamma = U\Lambda W^\top$ on the circular Brownian motion $\{\beta_t\}$. Obviously, $\varphi_t = W^\top \beta_t$ is still a circular Brownian motion, only started at a different point on the unit circle. Hence, $\Lambda W^\top \beta_t = (\lambda_1 \cos \varphi_t, \lambda_2 \sin \varphi_t)^\top$ is Brownian motion on the ellipse $\mathcal{E}(\Lambda)$ (Øksendal [18]). Finally, the action of the orthogonal matrix U is to map the ellipse $\mathcal{E}(\Lambda)$ onto the ellipse $\mathcal{E}(\Gamma)$, so that $U\Lambda W^\top \beta_t$ is still Brownian motion on an ellipse, only now on the ellipse $\mathcal{E}(\Gamma)$.

Finally, β_t is a Brownian motion on the unit circle, thus satisfying the Itô stochastic differential equation

$$d\beta_t = -\frac{1}{2}\beta_t dt + A\beta_t dB_t.$$

Applying Itô's lemma to the process $\{\Gamma\beta_t\}$ and noticing that Γ is of full rank, one has

$$dS_t = -\frac{1}{2}S_t dt + \Gamma A \Gamma^{-1} S_t dB_t,$$

and the proof is complete. \square

Remark 1. *The shape (eccentricity) and orientation of the ellipse $\mathcal{E}(\Gamma)$ characterizes the Kendall shape of the triangle V up to reflections.*

To see this, we notice that $V^\top V$ describes the shape-and-size of V , i.e. all those characteristics of V that are invariant under rotation and translation, up to a reflection. The entries of $V^\top V$ tell us about the norm of all the vertex vectors, and the pairwise angles they form but not the exact orientation of the vectors. Since Q is orthogonal, the same is also true for $\Gamma\Gamma^\top \equiv Q^\top V^\top V Q$, so that $\Gamma\Gamma^\top$ encodes the shape-and-size of the triangle V , up to reflections (complete knowledge of the initial shape-and-size requires knowledge of the sign of $\det(\Gamma)$). The shape of the triangle V is encoded in

$$\sigma(V) = \frac{\Gamma\Gamma^\top}{\text{tr}(\Gamma\Gamma^\top)},$$

along with the sign of $\det(\Gamma)$, the latter distinguishing between reflections. To make the connection between $\sigma(V)$ and $\mathcal{E}(\Gamma)$ clearer, we use the singular value decomposition of $\Gamma = U\Lambda W^\top$ (equation (4)). When Γ acts on the plane, it transforms the unit circle into the ellipse $\mathcal{E}(\Gamma)$. The major and minor axes of this ellipse are multiples of the columns of U . The lengths of these axes are given by twice the entries of Λ . Since the trace of a matrix is invariant under a similarity transformation, we may re-write $\sigma(V)$ as

$$\sigma(V) = \frac{U\Lambda^2 U^\top}{\lambda_1^2 + \lambda_2^2}.$$

Knowledge of the ellipse $\mathcal{E}(\Gamma)$ will thus provide the diagonal entries of Λ^2 (through the length of its half-axes of the ellipse) and the matrix U (through the orientation of the axes of the ellipse). Hence $\mathcal{E}(\Gamma)$ is a parametrization of the shape $\sigma(V)$ of V , up to a reflection. Conversely, the shape $\sigma(V)$ of V uniquely defines a “directed” ellipse of unit area. Notice that $\sigma(V)$ is a positive definite symmetric matrix, so that it admits an eigen-decomposition

$$\sigma(V) = D\Psi D^\top.$$

The square roots of the diagonal elements of Ψ will lead to the lengths of the half-axes of this ellipse. The orientation of its principal axes will be given by the matrix D . Finally, the “direction” will be given by the sign of $\det(\Gamma)$.

Summarising, we have seen that as the initial triangle V is rotated according to a Brownian motion modulo 2π , the shape-and-size of its projection $S(p(V, \beta_t))$ performs Brownian motion on an ellipse, whose characteristics (eccentricity and orientation) are in bijective correspondence to the Kendall shape $\sigma(V)$ of the original triangle V , modulo reflections. The actual *shape* of the projection $\sigma(p(V, \beta_t))$ will be a process on the unit circle, since Σ_1^3 is metrically \mathbb{S}^1 . If $w \in \mathbb{S}^1$, let $u(w) = (\cos w, \sin w)^\top$ be its extrinsic (Cartesian) representation. Let $\rho(w, \Gamma) = \|\Gamma^{-1}u(w)\|^{-1}$ be the norm of a vector lying on the ellipse $\mathcal{E}(\Gamma)$, whose argument is w . Then, we derive the following result:

Theorem 2. Let V be a proper planar triangle and $\beta_t = e^{iB_t}$ be circular Brownian motion, where B_t is standard Brownian motion in \mathbb{R} . Then, the shape $\sigma_t \equiv \sigma(p(V, \beta_t))$ of the Radon process $p(V, \beta_t)$, evolves as a diffusion process on the unit circle \mathbb{S}^1 , solving the Itô stochastic differential equation

$$d\sigma_t = \frac{\det(\Gamma)}{\rho^2(\sigma_t, \Gamma)} u(\sigma_t)^\top \Gamma A \Gamma^{-1} u(\sigma_t) dt - \frac{\det(\Gamma)}{\rho^2(\sigma_t, \Gamma)} dB_t. \quad (5)$$

We call the diffusion $\{\sigma_t\}_{t \geq 0}$ a *Radon diffusion of shape*.

Proof. Let $g : \mathbb{R}^2 \mapsto \mathbb{S}^1$ be defined by $(x, y)^\top \mapsto \arg(x, y)$ where,

$$\arg(x, y) = \begin{cases} \arctan(\frac{x}{y}), & \text{if } x \geq 0; \\ \arctan(\frac{x}{y}) + \pi, & \text{if } x < 0, y \geq 0; \\ \arctan(\frac{x}{y}) - \pi, & \text{otherwise.} \end{cases}$$

Then g is twice continuously differentiable, so that we may apply Itô's lemma to $g(S_t)$ and see that $\sigma(t)$ will be an Itô process satisfying the SDE

$$d\sigma_t = \frac{S_t^\top \Gamma A \Gamma^{-1} S_t S_t^\top (\Gamma A \Gamma^{-1})^\top A S_t}{\|S_t\|^4} dt - \frac{\det(\Gamma)}{\|S_t\|^2} dB_t. \quad (6)$$

Letting $u(\sigma_t)$ be the extrinsic representation of σ_t ,

$$u(\sigma_t) = \frac{S_t}{\|S_t\|},$$

and noting that $(\Gamma A \Gamma^{-1})^\top A = \det(\Gamma)(\Gamma \Gamma^\top)^{-1}$, the result follows by accordingly manipulating equation (6) \square

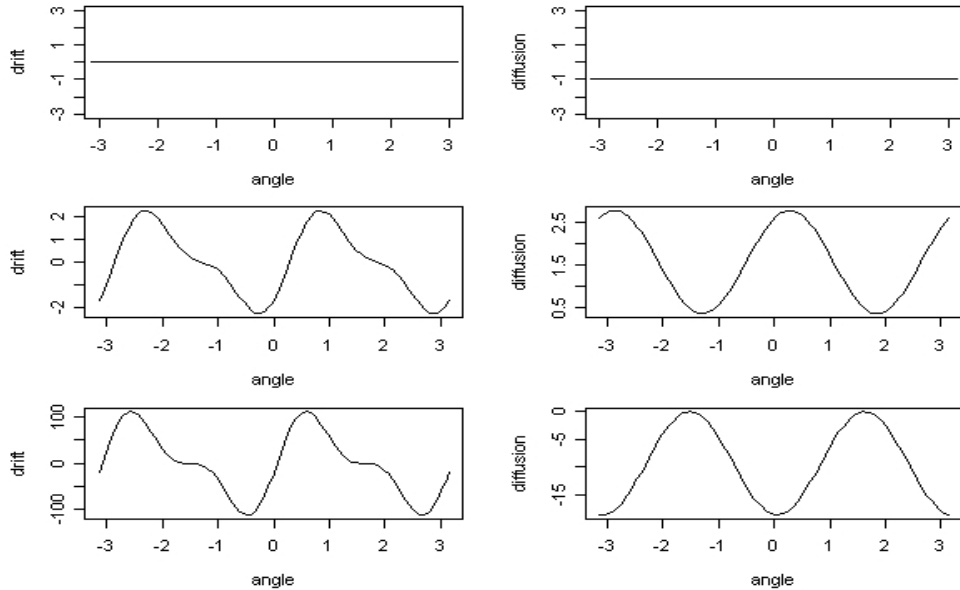


Figure 1: Drift and Diffusion coefficients for three different triangles. Each row corresponds to different triangle: an equilateral triangle, a “mildly” obtuse triangle, and a “very” obtuse triangle, respectively. Notice that the scale of the axes differs across different plots.

The differential equation (5) is revealing as far as the behavior of the Radon shape diffusion is concerned. It suggests that there are two “accumulation points” that are antipodal on the circle - the angles corresponding to the points of intersection of the unit circle by the major axis of the ellipse $\mathcal{E}(\Gamma)$. By the form of the coefficients, we can see that the process spends more time close to these points than elsewhere in the circle. In particular, both coefficients of the process at any point θ are inversely scaled by the squared norm of the point on $\mathcal{E}(\Gamma)$ with angular component θ . It is also interesting to note that the drift and diffusion coefficients remain unchanged if we multiply Γ by a constant, and so are invariant under scaling of the original triangle. Figure 1 contains some plots of the drift and diffusion coefficients on the interval $[0, 2\pi)$.

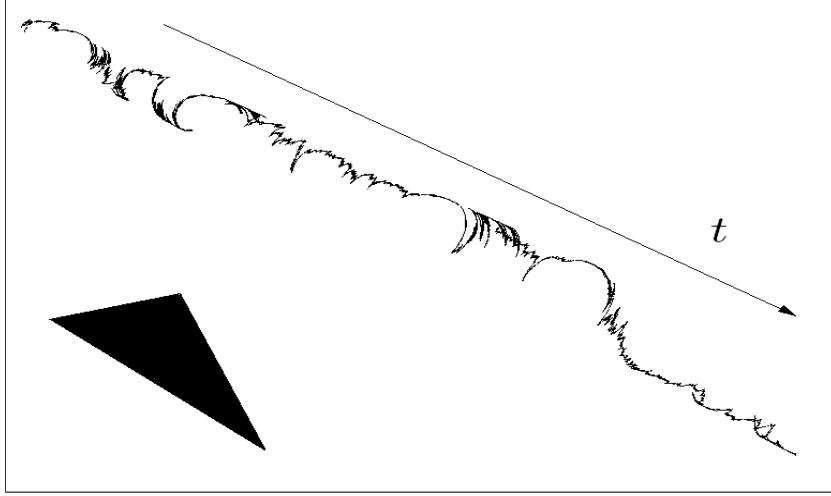


Figure 2: Sample path of a Radon shape diffusion. The process is plotted on a cylinder whose base is the unit disc, and the dimension corresponding to height is time. The triangle inducing the process is depicted on the lower left corner. The arrow indicates the time dimension, so that the cylinder is sloping diagonally across the figure, and is presented in perspective view

The movement of the process can be related to the shape of the initial triangle, specifically to the characteristics of its angles. An equilateral triangle will correspond to a maximum entropy case, and the resulting process is a Brownian motion on the circle (no time change required). When the points of the triangle approach collinearity the process tends to be heavily “attracted” by its accumulation points. In these cases, the process behaves somewhat like a random dynamical system, spending most time at two “attractors” (the antipodal points on the circle), so that when the process leaves any of these two points, it will quickly return to one of the two. Figure 2 and Figure 3 depict sample paths of Radon shape diffusions corresponding to two different planar triangles: a “mildly obtuse” triangle and a “very obtuse” triangle, respectively. We observe that in the ‘mildly obtuse’ case, the process is quite variable, although we may notice that the process tends to spend more time around two antipodal accumulation points. In the second case, the process spends most of its time close to its accumulation points, and these are easy to distinguish.

Generally, both the location of the accumulation points and the variability of the sample paths will depend on the shape of the initial triangle. In certain special cases, this relationship becomes more transparent. For example, all isosceles triangles with labels $\{a, b, c\}$ such that $ba = bc$ and $ba > ac$ will give the same accumulation points, regardless of the height of b . However, as the angles $b\hat{a}c = b\hat{c}a$ tend to become right angles, the variability around these accumulation points decreases.

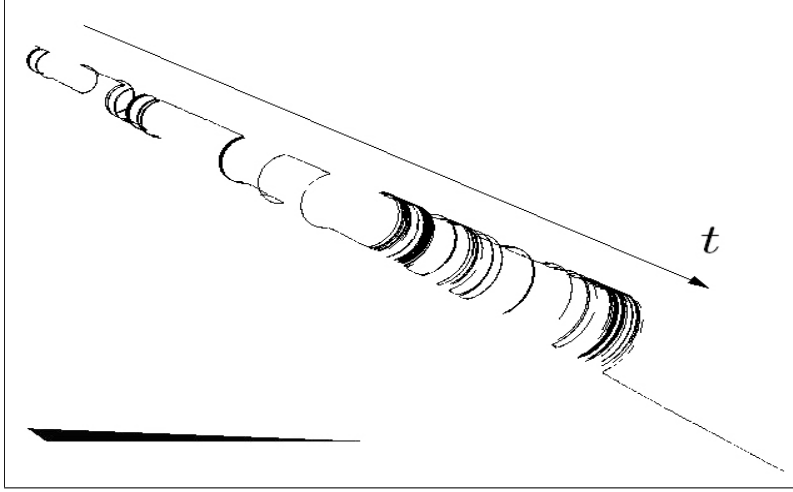


Figure 3: Sample path of a Radon shape diffusion, where the triangle inducing the process (depicted on the lower left corner) is “very” obtuse.

4 Stationary Distributions

If $\{\beta_t\}$ is Brownian motion on the unit circle started at angle $\beta_0 = 0$, then the density of $\vartheta_t := \arg(\beta_t)$ exists and admits the Fourier representation (e.g. Hartman & Watson [5]):

$$f(\vartheta, t) = \frac{1}{2\pi} \left\{ 1 + 2 \sum_{k=1}^{\infty} e^{-k^2 t} \cos(k\vartheta) \right\}, \quad \vartheta \in (-\pi, \pi].$$

Letting $\mu_t := \text{dist}(\vartheta_t)$, it follows by Scheffé’s theorem ([22]) that, as $t \rightarrow \infty$, μ_t converges to the uniform measure on $(-\pi, \pi]$ in total variation norm. This will also be the stationary distribution for ϑ .

Since the Radon shape diffusion $\{\sigma_t\}$ is obtained as a continuous function of $\arg(\beta_t)$, say $H(\arg(\beta_t))$, it follows that σ_t will weakly converge. The limiting distribution will be that of a random variable $X = H(\Theta)$, where Θ is uniformly distributed on $(-\pi, \pi]$.

In fact, we may force $\{\sigma_t\}_{t \geq 0}$ to be (strongly) stationary to begin with, so that $F := \text{dist}(X)$ is the marginal distribution of σ_t for all $t \geq 0$. To do this, we simply use a (strongly) stationary circular Brownian motion defined as

$$\tilde{\beta}_t := e^{i\tilde{B}_t}, \quad \forall t \geq 0,$$

where $\{\tilde{B}_t\}_{t \geq 0}$ is Brownian motion on \mathbb{R} , with initial distribution $\mathcal{U}(-\pi, \pi]$. We may thus determine the stationary distribution of the Radon shape diffusion from first principles.

Theorem 3. *Let V be a proper planar triangle and $\{\beta_t\}$ be circular Brownian motion. Then, there exists a stationary distribution F for the Radon shape diffusion $\sigma(p(V, \beta_t))$, having density f with respect to Lebesgue measure on $(-\pi, \pi]$, with*

$$f(\theta) = \frac{1}{2\pi} \frac{\rho^2(\theta, \Gamma)}{\lambda_1 \lambda_2}, \quad \theta \in (-\pi, \pi], \quad (7)$$

where λ_1, λ_2 are as before (equation (4)).

Proof. The discussion leading to the statement of the theorem settles the existence part of the proof. We thus have to show the validity of relation (7).

First, consider the case where the ellipse $\mathcal{E}(\Gamma)$ has its principal axes lying on the coordinate axes of the plane, so that U is the identity matrix. In particular, assume that

$$\mathcal{E}(\Gamma) = \left\{ (x, y) \in \mathbb{R}^2 : \frac{x^2}{a^2} + \frac{y^2}{b^2} = 1 \right\}.$$

If Θ is a uniform random variable on $(-\pi, \pi]$, we wish to determine the distribution of the random variable $H(\Theta) = \arg(a \cos \Theta, b \sin \Theta)$. That is, the distribution we wish to find is that of the angular component of a point $(a \cos \Theta, b \sin \Theta)^\top$ on the ellipse $\mathcal{E}(\Gamma)$.

To this aim, we first determine a folded version of this distribution and then proceed to unfold it. To be more precise, consider the random variable

$$Y = \arctan \left(\frac{b}{a} \tan \Theta \right).$$

This mapping provides the angular component of $(a \cos \Theta, b \sin \Theta)^\top$ modulo π , in the sense that it does not distinguish between angles that are π radians apart, giving values in $(-\pi/2, \pi/2]$.

When $\Theta \sim \mathcal{U}(-\pi, \pi]$ it is not hard to see that $\tan \Theta$ will have the standard Cauchy distribution, so that $Z = a \tan \Theta / b$ will have a distribution in the Cauchy family with density

$$f_Z(z) = \frac{a}{b\pi} \frac{1}{1 + \left(\frac{a}{b}z\right)^2}.$$

The distribution of $Y = \arctan Z$ can be seen to have density

$$f_Y(y) = \frac{a}{b\pi} \frac{1 + \tan^2 y}{1 + \left(\frac{a}{b}\right)^2 \tan^2 y} = \frac{1}{ab\pi} \frac{a^2 b^2}{b^2 \cos^2 y + a^2 \sin^2 y} = \frac{1}{\pi} \frac{\rho^2(y, \Gamma)}{ab},$$

for $y \in (-\pi/2, \pi/2]$. Finally, recalling our definition of $\arg(x, y)$, we see that the distribution of the random variable $H(\theta)$ has the density

$$f_0(y) = \frac{1}{2\pi} \frac{\rho^2(y, \Gamma)}{ab}, \quad y \in (-\pi, \pi].$$

This completes the proof for the case of an ellipse with principle axes falling on the coordinate axes of the plane. To move to the general case, we simply have to *rotate* this distribution according to the angle that the major axis of the ellipse forms with the x -axis. In particular, $\Gamma = U\Lambda W^\top$, and U gives the orthogonal transformation we have to perform to obtain the ellipse $\mathcal{E}(\Gamma)$ from the ellipse $\mathcal{E}(\Lambda) = \{(x, y) \in \mathbb{R}^2 : x^2/\lambda_1^2 + y^2/\lambda_2^2 = 1\}$. Orthogonally transforming the density according to U gives

$$f(y) = f_0(U^\top u(y)) = \frac{1}{2\pi} \frac{\rho^2(U^\top u(y), \Lambda)}{\lambda_1 \lambda_2}, \quad y \in (-\pi, \pi].$$

where $u(\theta) = (\cos \theta, \sin \theta)^\top$ and $\rho(u(\theta), \cdot) \equiv \rho(\theta, \cdot)$. Recalling the definition of $\rho(y, \Gamma)$,

$$\begin{aligned} f(y) &= \frac{1}{2\pi} \frac{1}{\lambda_1 \lambda_2 \| \Lambda^{-1} U^\top u(y) \|^2} \\ &= \frac{1}{2\pi} \frac{1}{\lambda_1 \lambda_2 (u(y)^\top U \Lambda^{-1} W^\top W \Lambda^{-1} U^\top u(y))} \\ &= \frac{1}{2\pi} \frac{\rho^2(y, \Gamma)}{\lambda_1 \lambda_2}, \end{aligned}$$

which proves that the function (7) is indeed the stationary density. \square

The intuition in the proof (that is perhaps obscured by the details of the derivation) is that we map a circular uniform random variable onto an ellipse. Then we project back onto the unit circle. Only both steps have been combined into a single step.

Remark 2. *The stationary density for the Radon shape process of a planar triangle belongs to the family of angular central Gaussian distributions (also known as offset normal or projected normal distributions).*

To see this, we recall the definition of this family (e.g. Mardia [16]),

Definition 2. Let G be a positive-definite symmetric 2×2 matrix. The central angular Gaussian distribution on the unit circle \mathbb{S}^1 with parameter matrix G is defined as the distribution having density with respect to Lebesgue measure on \mathbb{S}^1

$$f(y; G) = \frac{1}{2\pi} \det(G)^{-1/2} (u(y)^\top G^{-1} u(y))^{-1}, \quad y \in \mathbb{S}^1. \quad (8)$$

If we set $G = \Gamma\Gamma^\top$, we see that (7) is of the form (8). This family was introduced by Klotz [12] on the unit circle, while Tyler [23] considered the case for general hyperspheres (see also Watson [25]). Watson [24] used the central angular Gaussian to model rock deformations in geology. The name for this family comes from the fact that it can be obtained as the projection on the unit circle of a bivariate Gaussian distribution with variance-covariance matrix G (or indeed any distribution with G -elliptic contours). It is immediate from this representation that the matrix parameter $\Gamma\Gamma^\top$ is identifiable only up to scalar multiples, so that the stationary distribution depends only on the shape of the original triangle, modulo reflections.

This result is noteworthy in a couple of ways. First, it provides an explicit connection between the central angular Gaussian distribution and a particular diffusion on the circle, indeed a diffusion of *shape*. By the term “explicit” it is meant that the central angular Gaussian is the limiting distribution of this process (in fact, since the process can be made stationary to begin with, it is also the marginal distribution of this process in stationarity). Another connection with a diffusion is with planar Brownian motion, through the hitting time of the unit circle, and is as follows. If $\arg(B_t)$ is the angular component of a planar Brownian motion started at some point (r_0, θ_0) satisfying $r_0 < 1$, then $\arg(B_T)$ has a *circular Cauchy distribution* (e.g. Mardia [16]), where $T := \inf\{t \geq 0 : \|B_t\| = 1\}$ (e.g. McCullagh [17]). Hence, if we start the Brownian particle on the straight line $\lambda u(\theta_0)$ at a distance r_0 from the origin, the distribution of $\arg(B_T)$ will be of an angular central Gaussian type, since the circular Cauchy distribution can be easily obtained by folding the angular central Gaussian distribution.

More importantly, returning to our initial problem, we may use the knowledge of the stationary distribution of the Radon shape process in order to estimate the shape of the initial triangle, if only a finite sample path of $\{\sigma_t\}$ is at hand, thus providing a *statistical inversion* of the Radon shape diffusion (drawing an analogy with the inversion of the Radon transform). Of course, statistical inversion through the stationary distribution will never recover precisely the shape of the true triangle, but will estimate it up to a reflection. This is because the projection of a triangle V at angle ϕ is the same as the projection of the reflection of V at angle $-\phi$. Intuitively, the information given to us by the stationary distributions on the shape-and-size of the initial triangle comes from the location of its modes and by the spread. However, since the stationary distribution is symmetric, it does not allow us to distinguish between reflections.

5 The Singular Case

Consider the case in which the vertices of V are contained in a single straight line, so that the triangle is not proper (we will call it *degenerate*). Assuming again that the triangle is centered at zero (its centroid is zero), we have that its vertices are collinear. As a result, the matrix V has rank 1, so that Γ is singular. Hence, Γ maps the unit circle to a segment of the straight line defined by either of its columns (say the first one, to be denoted by γ), that is, a degenerate ellipse. This segment is “centered” at zero, and its length is equal to twice the single singular value in the singular value decomposition of Γ ,

$$\Gamma = U \begin{pmatrix} \lambda & 0 \\ 0 & 0 \end{pmatrix} W^\top.$$

Proposition 1. Let V be a degenerate planar triangle and $\beta_t = e^{iB_t}$ be circular Brownian motion, where B_t is standard Brownian motion. Then, the shape-and-size $S_t \equiv S(p(V, \beta_t))$ of the Radon process $\{p(V, \beta_t)\}$ evolves as $\lambda \cos B_t$ on the line segment $\ell(\gamma, \lambda) := \{\mathbf{x} \in \mathbb{R}^2 : \mathbf{x} = \alpha\gamma/\|\gamma\|, \alpha \in [-\lambda, \lambda]\}$.

Proof. This follows immediately from the singular value decomposition of Γ , through the application of Itô’s formula. \square

The resulting shape process will be slightly peculiar, in fact not well defined in terms of *shape*. The reason for this is that the state-space of the shape-and-size diffusion contains the origin. This means, that whenever S_t hits $(0,0)^\top$, the shape σ_t is *undefined* (in the words of D.G. Kendall, “from one point of view [coincident points] have no shape, and from another they ‘almost’ have every shape”). Thus the state space of the shape process contains three states: the states θ and $-\theta$ corresponding to the points of the unit circle that intersect with $\ell(\gamma, \lambda)$, and a state ϵ corresponding to undefined shape. In fact, the hitting times of the ϵ -state bear a resemblance to the zero set of Brownian motion in \mathbb{R} . If

$$\mathcal{T} := \{t \geq 0 : \sigma_t \in \epsilon\}$$

it follows that

$$\mathcal{T} = \bigcup_{m \in \mathbb{Z}} \left\{ t \geq 0 : B_t = \frac{\pi}{2} + m\pi \right\}.$$

As a result, \mathcal{T} is an uncountable set that has no isolated points with probability 1. It is also a set of measure zero.

We may think of the behaviour of σ_t once it has hit ϵ in terms of the behaviour of Brownian motion at zero. The ϵ -state will correspond to 0 while θ and $-\theta$ will correspond to $(0, \infty)$ and $(-\infty, 0)$, respectively. Recalling Blumenthal’s 0-1 law (e.g. Kallenberg [7]) we see that once the process hits the state of undefined shape, there is an infinity of instantaneous transitions between the three states (consistent with the pattern $-\theta \leftrightarrow \epsilon \leftrightarrow \theta$) until the process settles at one of the two “proper states” for a non-zero time interval.

The situation described will be the same for any collinear ensemble of k points in n dimensions. Whenever it happens that the ensemble is normal to the projection hyperplane, the shape of the projection onto that hyperplane will be undefined. In all other cases, the shape of the projection will be one of two reflected shapes in Σ_{n-1}^k . The behaviour of the resulting process at the point of undefined shape will be directly similar to that arising in the planar case.

6 Radon Shape Diffusions on Σ_1^k

The case of Radon shape diffusions arising from planar triangles holds a special place amongst Radon shape diffusions arising from k points on the plane. This is because the triangular case contains most of the essence of the theory for Radon shape diffusions from general labelled planar ensembles.

In the general case, we have $k \geq 3$ labelled points on the plane, $\mathbf{x}_1, \dots, \mathbf{x}_k \in \mathbb{R}^2$, centred at zero. Assume that not all k are collinear. We arrange these as columns of a $2 \times k$ matrix M ,

$$M = \begin{pmatrix} \mathbf{x}_1 & \mathbf{x}_2 & \dots & \mathbf{x}_k \end{pmatrix}$$

and study the process $p(M, \beta_t)$, as $\text{BM}(\text{SO}(2))$ acts on the columns of M :

$$p(M, \beta_t) = M^\top \beta_t.$$

Since the centroid of the points $\mathbf{x}_1, \dots, \mathbf{x}_k$ is zero, we may again orthogonally transform M , multiplying from the right with an appropriate $k \times k$ orthogonal matrix Q_k , the generalization of the matrix Q from equation (1). This matrix maps the columns of M to a new set of vectors,

$$\mathbf{x}_0^* = 0, \quad \mathbf{x}_m^* = \frac{1}{\sqrt{m^2 + m}} [m\mathbf{x}_{m+1} - (\mathbf{x}_1 + \dots + \mathbf{x}_m)], \quad m = 1, \dots, k-1$$

Again, we do this since knowledge of the centroid and $k-1$ points suffices for the description of the ensemble. Accordingly, the shape-and-size and shape processes are given by

$$S(p(M, \beta_t)) = Q_k^\top M^\top \beta_t \equiv \Gamma_k \beta_t \quad \text{and} \quad \sigma(p(M, \beta_t)) = \frac{\Gamma_k \beta_t}{\|\Gamma_k \beta_t\|},$$

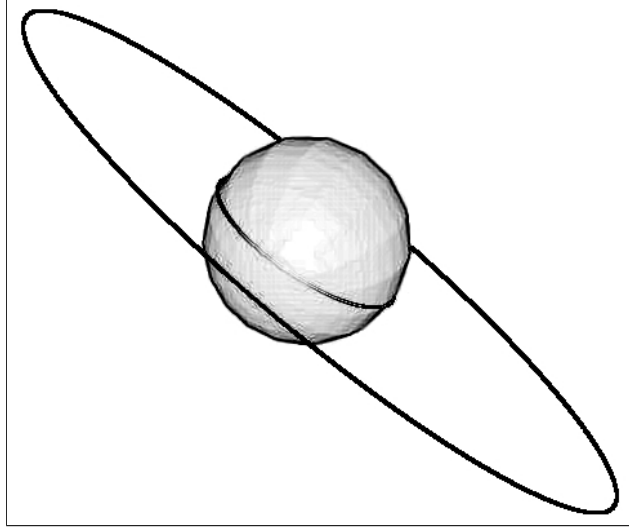


Figure 4: Representation of the range of motion of the Radon shape-and-size diffusion and the Radon shape diffusion when $k - 1 = 3$. The ellipse surrounding \mathbb{S}^2 is the range of the Radon shape-and-size diffusion, while the great circle on \mathbb{S}^2 is the range of the Radon shape diffusion.

respectively, where the $(k - 1) \times 2$ matrix Γ_k is defined analogously as before. Since we have assumed that not all k points are collinear, it must be that the matrix Γ_k has rank 2. As a result, Γ_k maps the unit circle \mathbb{S}^1 onto a (one-dimensional) ellipse in \mathbb{R}^{k-1} , say $\mathcal{E}(\Gamma_k) := \{\mathbf{x} \in \mathbb{R}^{k-1} : \Gamma_k \mathbf{y} = \mathbf{x}, \mathbf{y} \in \mathbb{S}^{k-1}\}$.

Specifically, we consider the singular value decomposition of Γ_k

$$\Gamma_k = H\Omega L^\top, \quad (9)$$

where H is a $(k - 1) \times 2$ matrix with orthogonal columns, $\Omega = \text{diag}\{\omega_1, \omega_2\}$ and L is a 2×2 orthogonal matrix. When Ω acts on the unit circle, it transforms it to the ellipse $\mathcal{E}(\Omega)$ on the plane. If one regards this plane as the plane $\{\mathbf{x} \in \mathbb{R}^{k-1} : x_m = 0 \forall m > 2\}$ (thus embedded in \mathbb{R}^{k-1}), the ellipse $\mathcal{E}(\Gamma_k)$ is obtained by orthogonally transforming $\mathcal{E}(\Omega)$. The orthogonal transformation is any element of $\mathcal{O}(k - 1)$ whose first and second columns are those of H .

Consequently, it can be seen that the Radon shape-and-size process is yet again a Brownian motion on an ellipse, namely on $\mathcal{E}(\Gamma_k)$. As a result, the Radon shape diffusion, will be a diffusion on a great circle of \mathbb{S}^{k-2} (obtained when projecting the ellipse $\mathcal{E}(\Gamma_k)$ onto \mathbb{S}^{k-2}). Figure 4 presents a schematic representation in the case $k - 1 = 3$.

It follows from our discussion that the stochastic differential equations for these diffusions and the associated stationary distributions for the case $k > 3$ can be obtained by an appropriate “rotation” of their counterparts in the case $k = 3$.

Theorem 4. *Let M be a k -ad of points in \mathbb{R}^2 , not wholly contained in any straight line. Let $\beta_t = e^{iB_t}$ be circular Brownian motion, where B_t is standard Brownian motion in \mathbb{R} . Then, the shape-and-size process $S_t \equiv S(p(M, \beta_t))$ is Brownian motion on the ellipse $\mathcal{E}(\Gamma_k)$ solving the Itô stochastic differential equation*

$$dS_t = -\frac{1}{2}S_t dt + \Gamma_k A(\Gamma_k^\top \Gamma_k)^{-1} \Gamma_k^\top S_t dB_t \quad (10)$$

Proof. Since the k -ad of points M in \mathbb{R}^2 are not wholly contained in any straight line, it will hold that Γ_k has rank 2. By the singular value decomposition of $\Gamma_k = H\Omega L^\top$, we have that

$$S_t = \Gamma_k \beta_t = H\Omega L^\top \beta_t.$$

Since L^\top is orthogonal, $L^\top \beta_t$ is a circular Brownian motion, so that $\Omega L^\top \beta_t$ is a Brownian motion on the ellipse $\mathcal{E}(\Omega)$. Finally, $H\Omega L^\top \beta_t$ is equal to $K\varepsilon_t$, where $K \in \mathcal{O}(k-1)$ is any orthogonal matrix whose first and second columns are those of H and $\varepsilon_t \in \mathbb{R}^{k-1}$ has all its coordinates zero, except for its first two coordinates, which correspond to the first and second coordinate of $\Omega L^\top \beta_t$, respectively. Hence $H\Omega L^\top \beta_t$ is Brownian motion on the one-dimensional ellipse $\mathcal{E}(\Gamma_k)$.

Now, let $g : \mathbb{R}^2 \mapsto \mathbb{R}^{k-1}$ be the mapping $x \mapsto \Gamma_k x$. Obviously, g is twice continuously differentiable, so that by Itô's formula, $S_t = g(\beta_t)$ is an Itô process satisfying the equation

$$dS_t = -\frac{1}{2}S_t dt + \Gamma_k A \beta_t dB_t,$$

where A is as before. But, Γ_k has rank 2 so that

$$S_t = -\frac{1}{2}S_t dt + \Gamma_k A (\Gamma_k^\top \Gamma_k)^{-1} \Gamma_k^\top S_t dB_t,$$

and the proof is complete. \square

Theorem 5. *Let M be a k -ad of points in \mathbb{R}^2 , not wholly contained in any straight line. Let $\beta_t = e^{iB_t}$ be circular Brownian motion, where B_t is standard Brownian motion in \mathbb{R} . Then, the shape process $\sigma_t \equiv \sigma(p(M, \beta_t))$ is a diffusion on the circle $\{\mathbf{x} \in \mathbb{S}^{k-2} : \mathbf{x} = \|\mathbf{y}\|^{-1} \mathbf{y}, \mathbf{y} \in \mathcal{E}(\Gamma_k)\}$, solving the Itô stochastic differential equation*

$$d\sigma_t = \left\{ -\frac{1}{2} + \eta(\sigma_t) H A H^\top \right\} \sigma_t dt - \det(\Omega) \frac{H A H^\top}{\|\Omega^{-1} H^\top \sigma_t\|^{-2}} \sigma_t dB_t,$$

where

$$\eta(\sigma) := \det(\Omega) \|\Omega^{-1} H^\top \sigma\|^2 \sigma^\top H \Omega A \Omega^{-1} H^\top \sigma$$

Proof. As noted earlier, the *shape* process will lie on a unit circle that is the projection of $\mathcal{E}(\Gamma_k)$ on \mathbb{S}^{k-2} . Consider the shape-and-size process on $\mathcal{E}(\Gamma_k)$. Intrinsically, this evolves as $\Omega \beta_t$, where $\Gamma_k = H\Omega L^\top$ is the singular value decomposition of Γ_k . When imbedded in \mathbb{R}^{k-1} , the process coordinates are given by $H\Omega \beta_t$, where the action of H is to rotate the 1-dimensional ellipse in space and place it at its “proper place”. A similar line of thought can be used to obtain the differential equation for the shape process. Intrinsically, this process will evolve as the shape process corresponding to shape-and-size $\Omega \beta_t$. Thus, in order to obtain the equation for σ_t , we only need to transform the shape process corresponding to $\Omega \beta_t$ according to H .

Let ψ_t be a diffusion on the unit circle solving equation (5) with Γ replaced by Ω . Let $g : \mathbb{S}^1 \rightarrow \mathbb{R}^{k-1}$ be $g(x) = H u(x)$, where $u(x) = (\cos x, \sin x)^\top$. Since g is twice continuously differentiable, Itô's formula applies to the process $\sigma_t = g(\psi_t)$ yielding the following differential equation for σ_t ,

$$d\sigma(t) = -\frac{1}{2}\sigma_t dt + H A u(\psi_t) d\psi_t. \quad (11)$$

Equation (5) gives the form for the differential $d\psi_t$,

$$d\psi_t = \frac{\det(\Omega)}{\rho^2(\psi_t, \Omega)} u(\psi_t)^\top \Omega A \Omega^{-1} u(\psi_t) dt - \frac{\det(\Omega)}{\rho^2(\psi_t, \Omega)} dB_t.$$

But H has orthogonal columns so that $\sigma_t = H u(\psi_t)$ implies that $H^\top \sigma_t = u(\psi_t)$, thus giving

$$d\psi_t = \frac{\det(\Omega)}{\|\Omega^{-1} H^\top \sigma_t\|^{-2}} \sigma_t^\top H \Omega A \Omega^{-1} H^\top \sigma_t dt - \frac{\det(\Omega)}{\|\Omega^{-1} H^\top \sigma_t\|^{-2}} dB_t.$$

If we plug this equation into equation (11) we obtain the desired result. This completes the proof. \square

Theorem 6. *Let M be a k -ad of points in \mathbb{R}^2 , not wholly contained in any straight line, and $\{\beta_t\}$ be circular Brownian motion. Then, there exists a stationary distribution F for the Radon shape diffusion $\sigma(p(M, \beta_t))$, having density f_k with respect to Lebesgue measure on $H\mathbb{S}^1$, with*

$$f_k(\mathbf{x}) = \frac{1}{2\pi} \det(\Gamma_k^\top \Gamma_k)^{-\frac{1}{2}} \{\mathbf{x}^\top (\Gamma_k \Gamma_k^\top)^{-1} \mathbf{x}\}^{-1},$$

where H is as before (equation (9)).

Proof. We have seen that σ_t evolves on a unit circle in \mathbb{R}^k , and that the intrinsic movement of the process is identical to that made by the process $\arg(\Omega\beta_t)$. Therefore, the stationary density of σ_t can be obtained by a suitable transformation of the density f given in (7). This transformation rotates the unit circle in $(k-1)$ -space. A short pause for thought reveals that $f_k(\mathbf{x}) = f(H^\top \mathbf{x})$, where f is the central angular Gaussian density with parameter matrix Ω . This completes the proof. \square

7 Discussion

In this paper, we have introduced a problem that combines concepts from stochastic geometry (D.G. Kendall shape) and integral geometry (Radon transform), motivated from a problem in biophysics (single particle electron microscopy). This is the problem of relating the shape of a planar configuration to the shape of its projections on random sets of lines. In particular, we have introduced a stochastic analogue of the Radon transform, essentially a Radon transform whose angular component is a stochastic process. Then, we proceeded to study the properties of Radon diffusions induced by planar configurations of labelled points, when the angular component evolves as a Brownian motion in the rotation group $\text{SO}(2)$. We obtained the stochastic differential equations and stationary distributions for the shape of such Radon processes. Special emphasis was given on the case where the planar ensemble was a triangle, as it was seen that this case contained the basic ingredients for the study of the general planar case. It was found that the characteristics of these Radon diffusions had immediate connections to the shape of the initial configuration of points, and that the stationary distributions of these diffusions were in bijective correspondence with the shape of the initial triangle, modulo reflections.

Further study of this problem may involve the consideration of the intrinsic differential geometry of Radon diffusions in the general scenario of k points in $n < k$ dimensions. The complexity of the geometry of general shape spaces Σ_n^k (see Kendall [9], Le & Kendall [15], Le [14]) makes such a study quite difficult, although some cases could be tractable. Nevertheless, using the so called *inner product coordinates* for shape and shape-and-size, certain basic results on the general case have been derived by the author (Panaretos [19]). In particular, necessary and sufficient conditions have been obtained for the recovery of the Brownian “orientation” process, from observation of the shape process and knowledge of the initial ensemble of points. Furthermore, it has been shown that, as with the planar case, the shape and shape-and-size processes in the general case are indeed diffusions, and their stationary distributions may be related to the unoriented shape-and-size of the initial ensemble. Finally, work in progress by the author (Panaretos [20]) focuses on the statistical aspects of Radon diffusions.

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